An Undulator Beamline for Protein Crystallography at the NSLS: Commissioning and Operation of X29

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Beam line X29 of the National Synchrotron Light Source (NSLS) has been operating for a year for macromolecular crystallography (PX) research, employing a mini-gap, in-vacuum undulator as its X-ray source. Development of this facility involved a close collaboration among the groups of Mark Chance (Case Proteomics Center, Case Western Reserve Univ. [CWR]), Erik Johnson [NSLS], and Robert Sweet (Macromolecular Crystallography Research Resource [PXRR] of BNL's Biology Dept.).

There were several joint objectives and complexities to this project. Firstly, we hoped to provide an undulator-based beam line with the attractive features of high collimation and high flux for macromolecular crystallography at the NSLS. This would complement the multiple dipole-based facilities and the wiggler source at X25. The new source would be the sort of in-vacuum, mini-gap undulator devised earlier by the NSLS and contemplated for synchrotron radiation facilities around the world, such as the Swiss Light Source and the Canadian Light Source. Whereas X25 has been used for the thorniest crystallographic problems, we hoped to optimize X29 for high throughput and rapid access. Secondly, X29 was one of the only remaining undeveloped straight sections of the X-ray ring, and its development for user science programs was considered essential to maintaining competitiveness for this second generation source [1].

The difficulties in developing this straight section included the presence of two large out-dated radio frequency (RF) cavities in this area of the ring, and available floor space that was very limited owing to the proximity of the ring injector. The design would have to be extremely parsimonious in its use of space. Thirdly, there was no clear source of funding. This project was begun at a time when there were many other beam lines being constructed at sources around the world, and there was the perception that a new one was not needed despite the dearth of insertion devices on the East Coast of the U.S. These challenges stimulated the formation of the above collaboration, which eventually received sufficient funding from the Biological and Environmental Research and Basic Energy Sciences offices of the U.S. Department of Energy, the National Institute for General Medical Sciences (NIGMS), the National Center for Research Resources, and the National Institute for Biomedical Imaging and Bioengineering of the U.S. National Institutes of Health. We believe the results have justified the funding of this project, even in this difficult funding environment.

Solutions

The key to development, commissioning, and now operation of this experimental station has depended on a close and collegial cooperation among the members of these groups. The division of responsibilities was that the NSLS would provide the source, new RF cavities, and all the apparatus inside the shield wall of the X-ray ring; CWR would specify, procure, and install all of the X-ray optics, delivery pipes, and the X-ray hutch; and the PXRR would do the same for the experimental station. In the end, from the approval of the construction of the beam line and experimental station itself in late 2002 to the official declaration of Operational Status in fall 2004, the project was on or ahead of schedule and on or below the budget. Here are some of the solutions chosen.

The X-ray Undulator. The quality and usefulness of a short (300 mm) mini-gap, in-vacuum undulator (MGU) had already been proven by the NSLS, and one was in use at beam line X13 [2, 3]. The NIH provided funds some years ago both to replace the RF cavities in the X29 straight section with modern, smaller ones, and to provide a short undulator, shown in Figure 1, which would fit in this space. The undulator

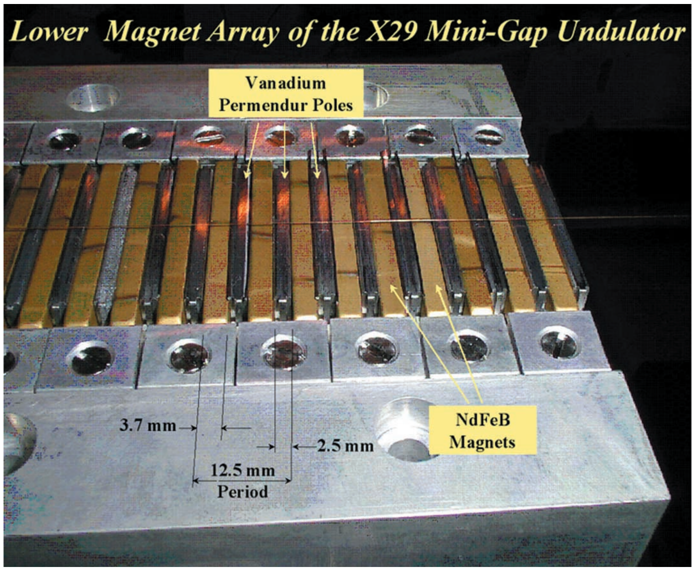

Figure 1: A section of the lower magnet array of the X29 minigap undulator. The device is 34 cm long, comprising 27 periods, each 12.5 mm.

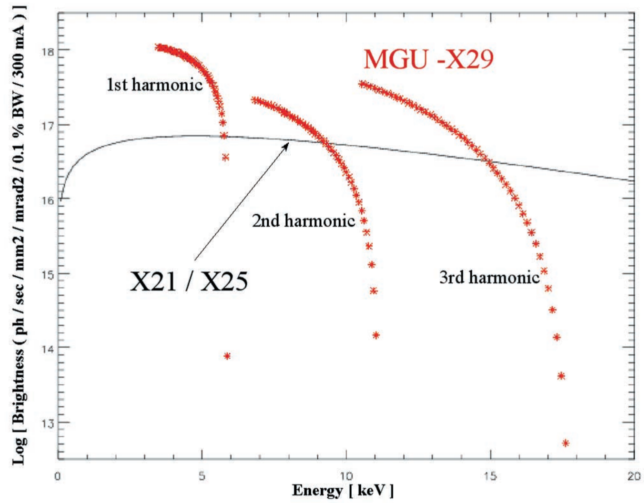

Figure 2: Calculated emission spectra for the X29 undulator compared to the X25 wiggler. The individual points for X29 are generated as the gap between the magnet assemblies is widened.

has been shown in theory and practice to produce the sort of emission spectrum shown in Figure 2. Although there is a gap between them, the curves for the second and third harmonics produce copious illumination in regions of the spectrum that are extremely useful for PX.

X-ray Optical System. The problem was to compress an entire optical system *and* experimental station into a very small space. One aspect of the solution was to move the shield wall upstream nearly six feet (see Figure 3), and to make it thinner by use of high density concrete. This allowed us to place the cryogenic monochromator outside the shield wall for easier installation and servicing.

The central components of the system are a double crystal monochromator with a sagittally bent second crystal, which provides horizontal focusing, followed by a cylindrically bent mirror that provides vertical focusing and harmonics rejection. This system provides independent focusing in horizontal and vertical directions, and allows one to focus on the sample or on the detector for optimal data acquisition. The photon energy range of the monochromator is 4–18 keV. The first monochromator crystal (Si-111) is cryogenically cooled by a refrigerator system that achieves temperatures near to 90 K to prevent distortions from the high-power density of the undulator emission. The second crystal is at room temperature. The 700-mm-long mirror, made of ULE (ultra-low thermal-expansion glass), has a Pd-coated, a Pt-coated, and an uncoated stripe, each of which can be translated into the beam for proper harmonics rejection without changing the mirror angle over the entire photon-energy range. The optical system is an adaptation of the system installed at sector 22-ID (SER–CAT) at the APS. However, owing to the extreme limitation of space, monochromator and mirror systems have been compressed into the same vacuum chamber. The horizontal demagnification ratio is 4.1:1, when focused on the sample, and 5.8:1 in the vertical direction. Beam sizes as small as 125 µm x 80 µm (FWHM, horizontal x vertical) have been achieved at the sample. However, beam sizes of 165 x 100 µm are commonly used. The most recently measured X-ray flux at the sample position through a 0.1 x 0.12 mm rectangular aperture is 5 x 10^{11} photons/sec at 1.1 Ång.

Diffractometer/Detector System. We chose an ADSC Q315 detector/diffractometer combination. This 315 mm-square CCD-based detector system gives near 100 µm resolution with near 2 sec readout. This has resulted in data collection times of ~5 sec per frame for many crystallographic problems. The diffractometer includes a fast (30 rpm) servo-motor ω drive with a "mini-κ" on top of a tripod-based motorized orienter. The mini-κ system allows one to flip the crystal mount to +50° from the horizontal for mounting a crystal from a vial of liquid nitrogen, or to change the axis of rotation.

Control. We have adopted components that allow modular development and servicing, but which can be gathered easily under a single monolithic control system for the user. The **cbass** software system communicates with the in-hutch motors and the NSLS undulator-gap system through EPICS (Experimental Physics and Industrial Control System http://www.aps.anl.gov/epics/), to the Compumotor diffractometer con-

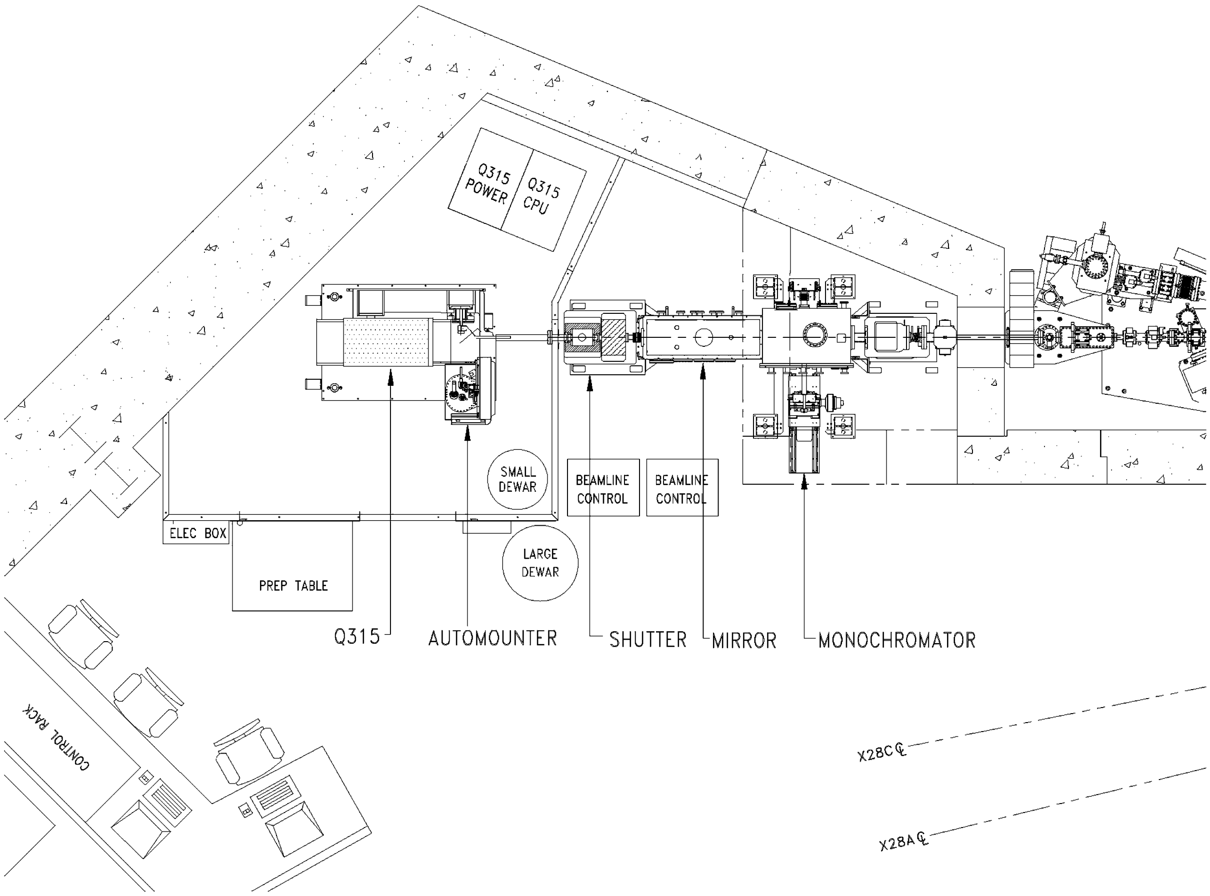

Figure 3: The layout of the X29 beam line. Notice that the shield wall has been moved almost six feet upstream to accommodate the cryogenic Si (111) monochromator, which is followed by the focusing mirror and the shutter.

trol (which has its own click-to-center routine), and to the CWR beam-line-control system. This approach allowed us to provide the user with transparent and rapid shifts in photon energy rather early in the commissioning process.

The Pathway to Improvement. From the beginning, we have employed an aggressive scheduling of the beam line use coupled to continuous development. "Prime time" during the week is used for development when there are improvements to implement. This provided the opportunity for rapid development of the real-time undulator control, which is the heart of the transparent energy changes. This allowed the CWR beam line staff to make continuous incremental improvements in focusing, enhancing the flux-density of the beam. This has allowed installation of a robotic crystal auto-mounter that is just now coming into operation, with little negative effect on the productivity.

Coordinated with aggressive development is tightly scheduled and well supported use of the beam line. Structures have been solved with only one-half hour of beam time, so although many users will visit for about a day, frequently one-project users will be booked in for 2–4 hours. Our local mail-in (FedEx project) scientists and the local structural genomics users from the NIH funded New York Structural Genomics Research Consortium have provided a cohort of regular and experienced users who are sensitive to every moving part of the system. They provide a constant critique of beam line hardware, operations, and scheduling that leads to continuous improvement. Both the PXRR and CWR have devoted a critical mass of scientific, engineering, and user-oriented staff to provide rapid response, both to users' problems and to possibilities for improvement. This sort of environment helps to drive other projects, for example robotics development, an experiment-tracking database, PXDB, and a continually evolving computation environment. The latter includes a massive disk farm and comfortable and convenient Cyber Cafés to which experimenters may retire to finish processing and archiving of data.

Effectiveness. X29 is a significant success and is hugely productive. On average more than one group per day visits to make measurements. Data collection times are comparable to Advanced Photon Source Undulator A crystallography stations. The flexibility of the station is such that data at 1-Å resolution have been measured, as have data from crystals with unit cells >600 Å. However the main emphasis of our work has been to provide eager and earnest support of users, and a “friendly” interface (both hardware and software) between the investigators and the experimental station. This allows a rapid interleaving of groups for short, stress-free, and productive visits. This facility, with its proximity to the large number of productive crystallography groups along the Atlantic Coast, is likely to be one of the most productive protein crystallography facilities in the world.

Acknowledgements

We are grateful for support from the United States Department of Energy Office of Biological and Environmental Research to the BNL Biology Department, and Office of Basic Energy Sciences to the NSLS, under DOE contract DE-AC02-98CH10886. We also are grateful for support from the United States National Institutes of Health National Center for Research Resources, grant P41-RR-012408 to the BNL Biology Department, the National Institute for Biomedical Imaging and Bioengineering Biomedical Technology Resource program, grant P41-EB-01979 originally to the Albert Einstein College of Medicine, and now to Case Western Reserve University, the National Institute of General Medical Sciences and NCRR grants N1-GM-9069-01 and Y1-RR-9004-01 to the NSLS, and NIGMS Protein Structural Initiative grant P50-GM-62529 to the New York Structural Genomix Research Consortium at Structural Genomix Inc.

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